



PARTNERSHIP
TO ADVANCE
COMBUSTION
ENGINES

ACE142: Development and Validation of Simulation Tools for Advanced Ignition Systems

Riccardo Scarcelli, Joohan Kim, Vyaas Gururajan (ANL)

Jacqueline H. Chen, Tuan Nguyen (SNL) – Shashank Yellapantula, Bruce A. Perry (NREL)

FY20 DOE Vehicle Technologies Office Annual Merit Review, June 2, 2020



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OVERVIEW

Timeline

- PACE start: FY 2019 Q3 (April 2019)
- PACE end: FY 2023 Q4 (September 2023)
- ≈ 25% Complete

Budget*

- Funding in FY19: \$400k
\$400k (PI: Scarcelli, C.02.04)
- Funding in FY20: \$875k
\$300k (PI: Scarcelli, C.02.04)
\$100k (PI: Scarcelli, C.02.04, FCA-CRADA)
\$100k (PI: Chen, C.02.01)
\$100k (PI: Nguyen C.02.03)
\$275k (PI: Yellapantula C.02.02)

Barriers

- Addressing PACE Major Outcomes 4,5,6,7,8
- Lack of predictive models for conventional and non-conventional ignition processes in engines
- Limited understanding of advanced ignition mechanisms that enable high-efficiency engines

Partners**

- PACE: Ignition Experiments (Ekoto, ACE141), Kinetics (Wagnon, ACE139 and Whitesides, ACE140), Cold-start (Curran, ACE149), Combustion (Ameen, ACE146)
- Convergent Science, Esgee Technologies
- Tenneco, Transient Plasma Systems (TPS)
- Michigan Tech, U-Texas, U-Perugia, Auburn, Purdue
- FCA Group (2-yr CRADA with DOE/ANL)

* As a reference for task numbers and PIs, Reviewers can check the attached 'Complete PACE Budget' slide

** PACE is a DOE-funded consortium of six National Laboratories working towards a common goal (ACE138). Goals and work plan are developed considering input from stakeholders including DOE, ACEC Tech Team, CFD code developers, and more.

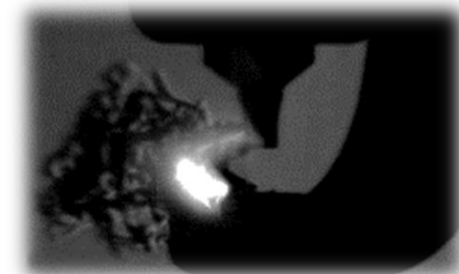
RELEVANCE/OBJECTIVES

The development of predictive ignition models is needed by Industry, and can leverage fast-growing high-performance computing resources

■ Conventional spark-ignition (SI)

- Several models available, tied to combustion/turbulence model of choice.
- Scarce validation at challenging operation (boosted high-load, lean/dilute).
- Unidentified issues at specific operation of interest to industry (e.g. cold-start).
- Missing components (electrical discharge, strikes/restrikes, conjugate heat transfer, radiative heat losses, plasma properties, etc.) negatively affect the model predictivity.

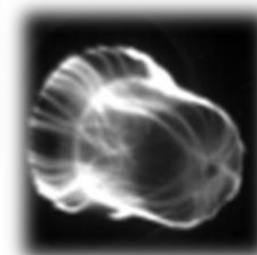
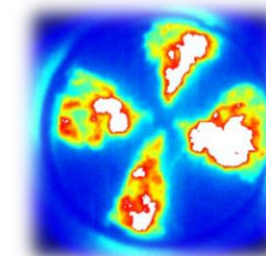
Image: MTU



■ Advanced ignition systems

- Spark-based systems (e.g. Pre-chamber, PC):
 - Leverage progress on SI. Additional complexities from unique challenges for PC.
 - Not purely an ignition modeling problem (the combustion model is also crucial).
- Alternative systems (e.g. low-temperature plasma, LTP):
 - No dedicated models offered by CFD tools. Simplistic energy/species deposition used.
 - Complex LTP chemistry, resulting in mechanism size not affordable for CFD calculations.
 - Additional complexity from lack of fundamental experiments. Model validation is challenging.

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Overall Relevance of PACE: PACE combines unique experiments with world-class DOE computing and machine learning expertise to speed discovery of knowledge, improve engine design tools, and enable market-competitive powertrain solutions with potential for best-in-class lifecycle emissions.

APPROACH

Combustion and Kinetics

Experiments and DNS of kernel growth
(SNL)

Predictive
Ignition Model

Plasma modeling
(ANL)

LES/RANS sub-models
(NREL, SNL, ANL)

CONVENTIONAL
SI

ADVANCED IGNITION SYSTEMS

PACE MAJOR OUTCOMES

- 4. High-load ignition models
- 5. Lean/dilute ignition models
- 8. Cold-start ignition models
- 6. Advanced Igniters
- 7. SI/ACI controls

DNS: Direct Numerical Simulations
LES: Large Eddy Simulations
RANS: Reynolds-Averaged Navier-Stokes
ACI: Advanced Compression Ignition

MILESTONES

Date	PI	Milestone	Status
FY19 Q3	Scarcelli	Validate LTP simulations from advanced LTP ignition technologies (i.e. TPI, GBDI, RF Corona) against experiments	100% Complete
FY20 Q2	Scarcelli	Expand ignition models to improve CFD predictions at dilute engine operation	50% Complete
FY20 Q2	Yellapantula	Assess ability of ML-based models to capture spatially filtered DNS heat release rates	90% Complete
FY20 Q2	Nguyen	Multi-zone CFD model analysis of early-state ignition	Delayed to Q4FY20
FY20 Q3	Chen	Perform DNS of turbulent kernel evolution with EGR dilution	On track
FY20 Q4	Scarcelli	Simulate the impact of advanced ignition concepts on ACI operation in CFD simulations	Rescheduled in FY21-23
FY20 Q4	Scarcelli	Model ignition at cold-start conditions using conventional computational methods	On track
FY20 Q4	Yellapantula	Evaluate turbulent-chemistry interaction model prediction against imaged spark kernels	On track
FY20 Q4	Nguyen	Mine statistics from comparable DNS to identify relevant early flame kernel model features	On track
FY20 Q4	Chen	Provide framework for extracting statistics from DNS for model development	On track

TPI: Transient Plasma Ignition
 GBDI: Groundless Barrier Discharge Ignition
 RF: Radio-Frequency

Ignition modeling tools (plasma, CFD, kinetics) improved and expanded

VizGlow/CONVERGE CFD

- ANL/EsGee Technologies long-established collaboration led to VizGlow improvements.
- LTP ignition model in CONVERGE expanded:
 - UDF source terms from VizGlow/Bolsig+
 - Output from VizGlow taken as input to CONVERGE and vice versa (on-going)



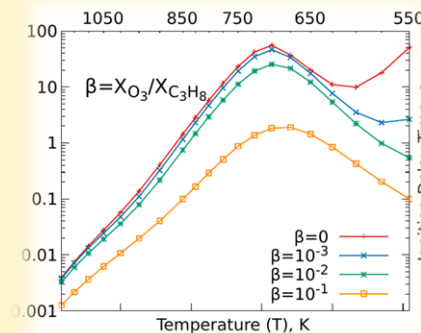
VizSpark/CONVERGE CFD

- Introduced high-fidelity SI modeling using VizSpark to evaluate plasma properties, spark stretch, blowouts, and re-strikes.
- ANL/EsGee Technologies new collaboration on 1-way coupling of VizSpark and CONVERGE (on-going).



0-D/1-D kinetics

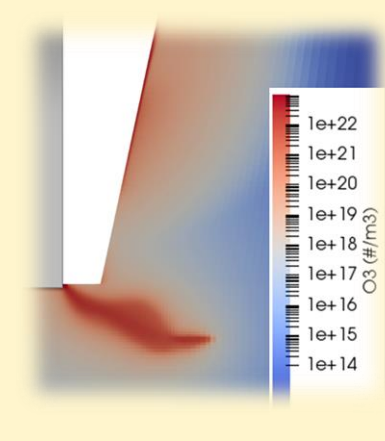
- 0-D modeling of impact of radicals on auto-ignition processes showed the importance of ozone (O_3).
- 1-D modeling of impact of radicals on flame propagation and kernel radius evaluated for different fuels (Le number effects).



Expanded Mechanisms

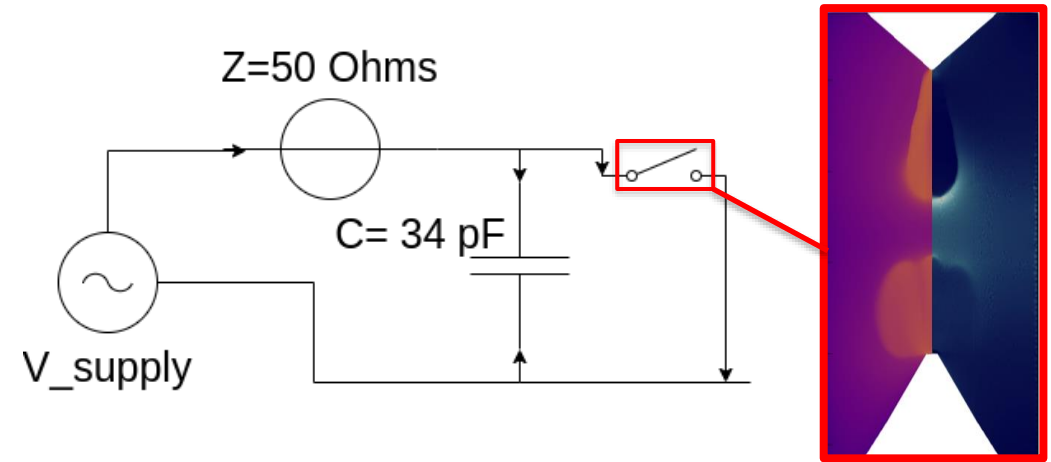
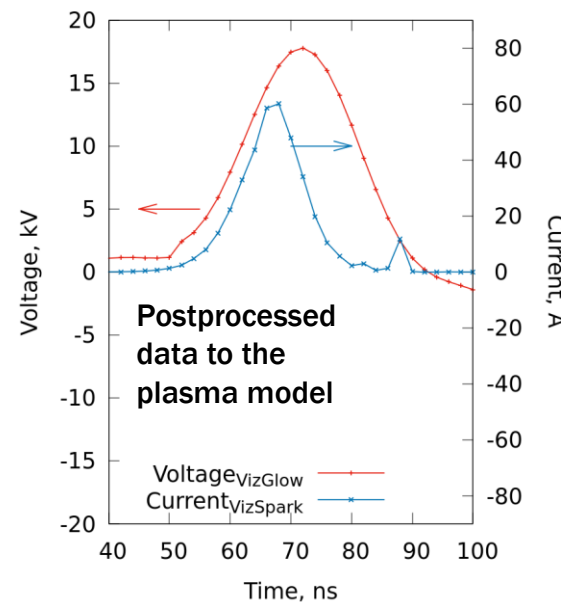
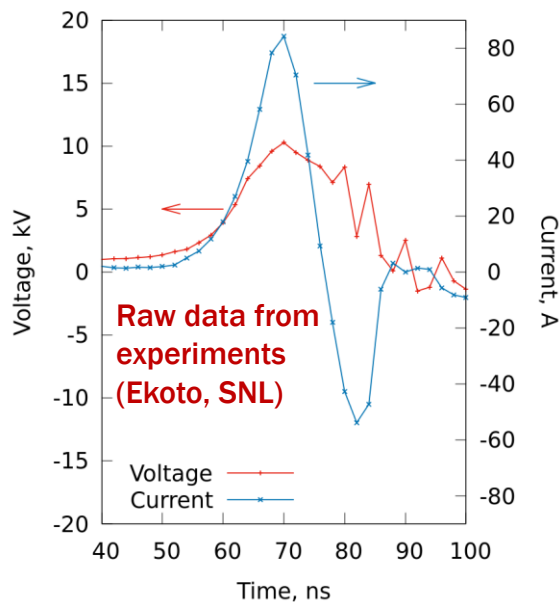
- Simplified O_3 kinetics added to the plasma mechanism used in VizGlow.
- Shown good agreement with SNL experiments (GBDI) for $[O_3]$:

Simulations	Experiments
$O_3 = 3.13$ ppm	$O_3 = 3.75$ ppm



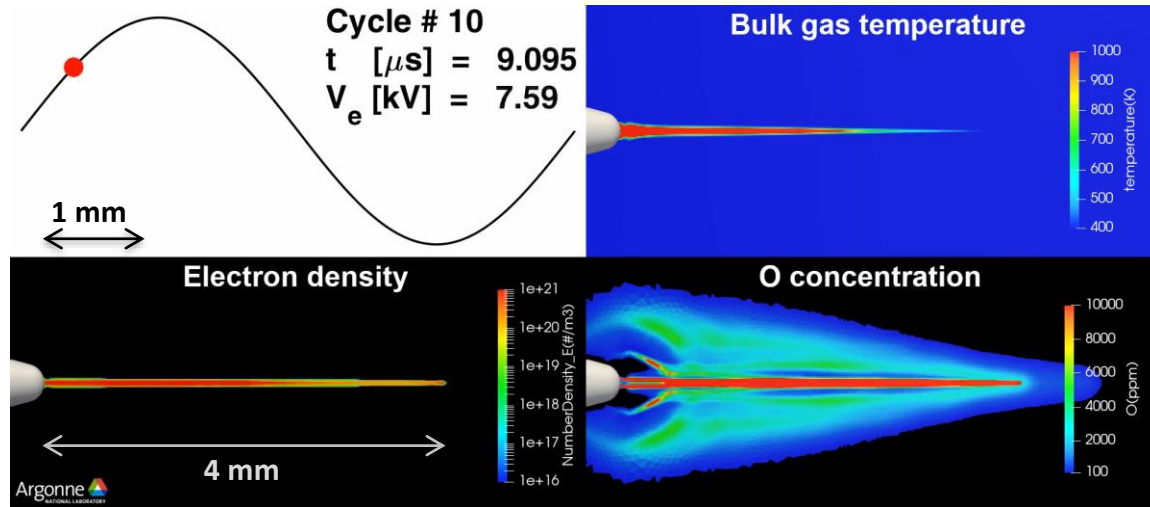
Improved characterization of discharge-to-plasma simulations

- Previously simplified boundary conditions required extensive tuning of the model to match experiments.
- Improved circuit calculations take transmission line losses into account.
- Circuit modeling calibrated with SNL experiments using the open source code Screamer. Collaboration with TPS under the HPC4Mfg program.



- Raw Voltage/Current data from SNL experiments was post-processed to obtain realistic values of:
 - Connection Voltage → VizGlow
 - Connection Current → VizSpark
 - Power dissipated into the gas → CONVERGE
 - Energy deposited into the gas → Cantera (0-D equilibrium calculations)

RF corona plasma simulated and validated against experiments



- Collaborative effort between ANL, U-Perugia, and Tenneco.
- Non-equilibrium plasma simulations using VizGlow captured the rapid succession of positive and negative streamers from a high-voltage RF discharge.
- Peak values in the range of $[O] = 5,000\text{-}20,000$ ppm and $\text{Temperature}_{\text{BULK}} = 1500\text{-}3000$ K, based on the operating conditions ($V_{\text{MAX}} = 13.5\text{-}19$ kV, Pressure = 3.25-5.5 bar).
- Case shown in this slide: 13.5 kV and 3.25bar

- Experimental trends at different V_{MAX} /Pressure ratios were captured.
- Quasi-steady streamer penetration was reached within 10-15 cycles and matched optical data from U-Perugia.

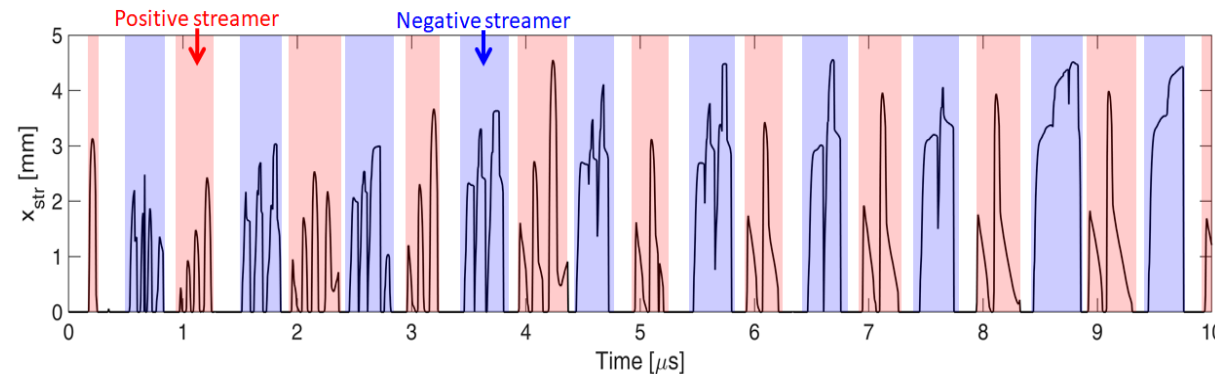
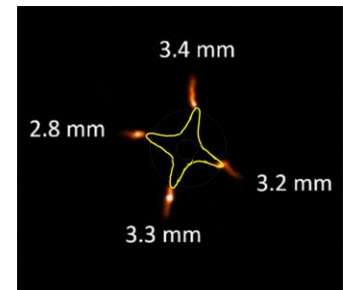


Image from U-Perugia



Milestone: Modeling capabilities developed for LTP advanced igniters (TPI*, GBDI*, Corona)

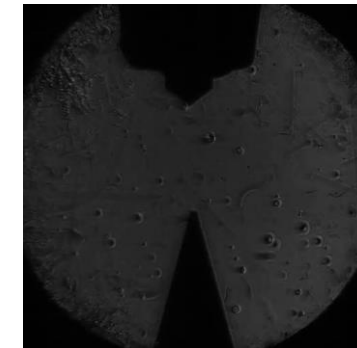
Engineering-level TPI model for CFD solvers developed

UDFs: User Defined Functions

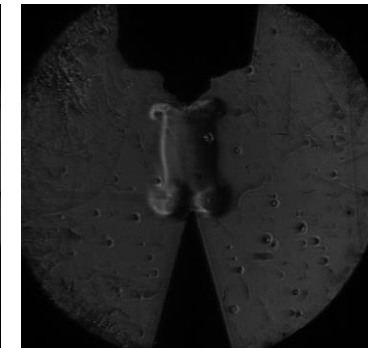
Pin-to-pin 2-pulse LTP ignition of propane/air mixture (Ekoto, SNL)

- **Objective:** canonical geometry and designed experiments (ignition with low number of pulses) are suitable for initial validation of the LTP ignition CFD model.
- 3.4 mm gap, $p = 1.3$ bar, $T = 343$ K, $\phi = 1.0$, 20 ns pulse, 300 μ s dwell time.
- Dissipated power from VizGlow fed into Bolsig+ to identify elastic/inelastic collision ratio. Calculated heat/species sourced in CONVERGE via UDFs.
- Flexible approach to tune thermal/chemical ratio for multiple pulses.
- CONVERGE LES + multi-zone finite rate chemistry.
- 1st pulse deposition does not heat up the gas.
- 2nd pulse deposition heats up the plasma due to larger elastic component.
- Removes previous assumption (i.e. same energy/species deposition at each pulse).
- Qualitatively captures 2nd pulse ignition.
- Pending validation with new dataset (methane).

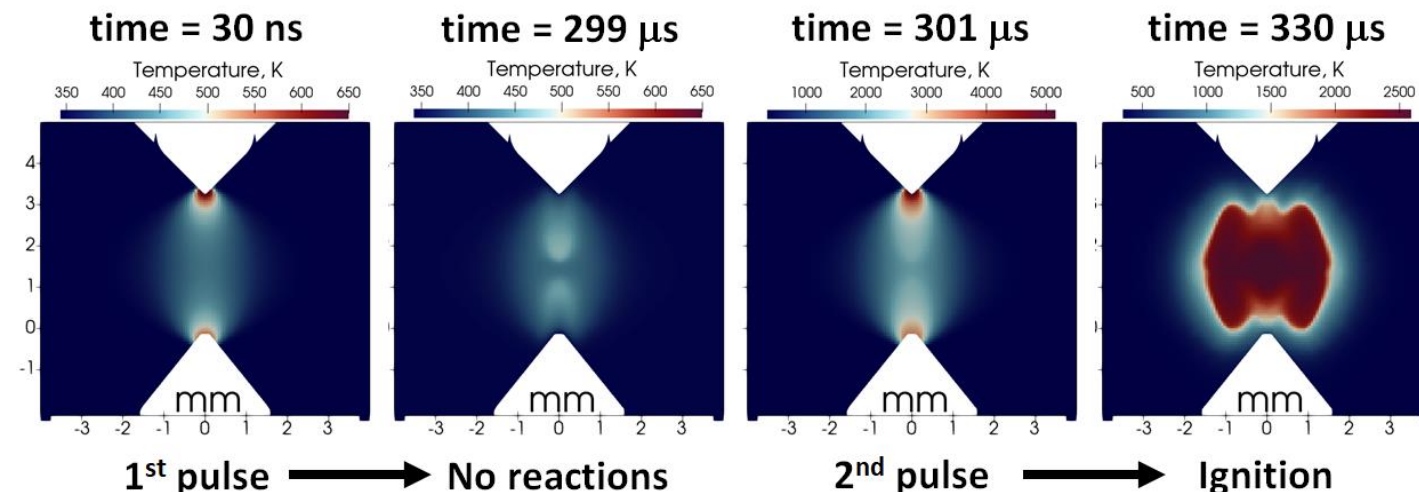
1st discharge



2nd discharge



Schlieren images from Ekoto, SNL

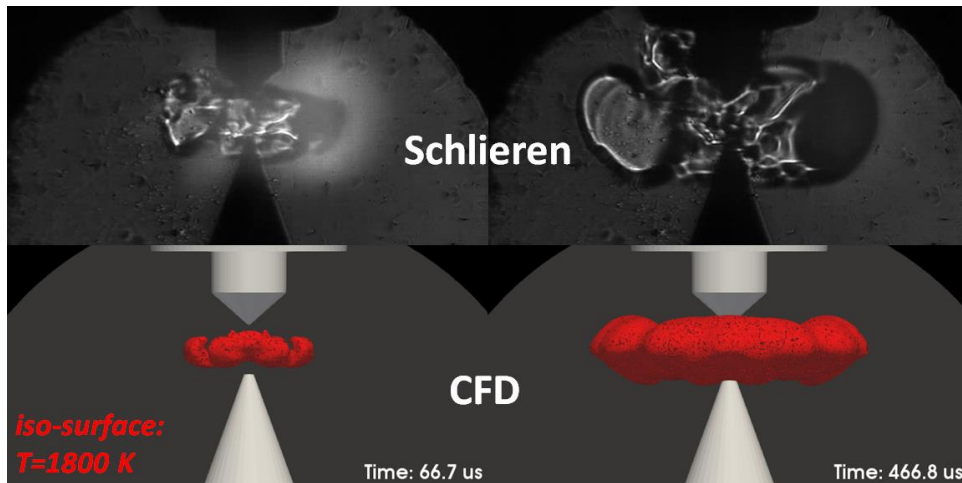


SI kernel growth simulated with CFD and compared with experiments

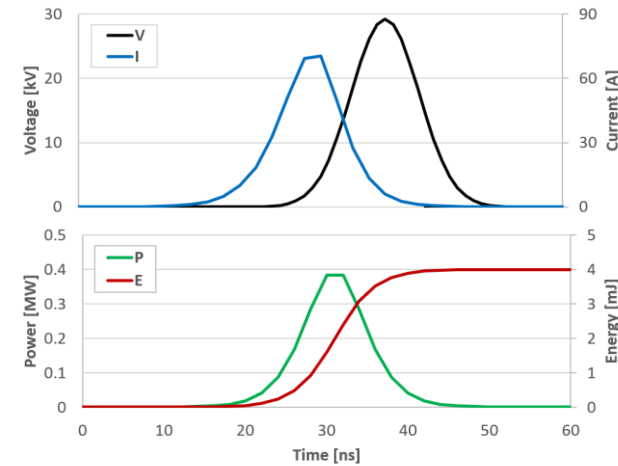
Pin-to-pin spark in methane/air mixture (Ekoto, SNL)

- **Objective:** designed experiments to decouple the spark-induced kernel growth from the electrical discharge.
- High-voltage nano-pulse (20 ns) resulting into a spark.
- Experiments at engine-like density: 5bar, 343 K.
- VizSpark for discharge-to-plasma simulations. Switched to CONVERGE after 50 ns for combustion calculations.

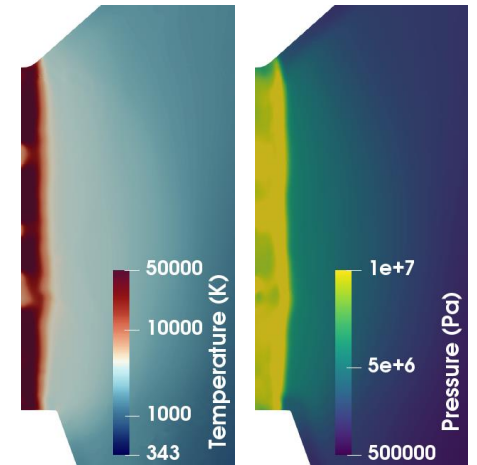
Schlieren images from Ekoto, SNL



Post-processed data to VizSpark



VizSpark output (t = 50 ns)



CONVERGE CFD results compared to Schlieren from SNL

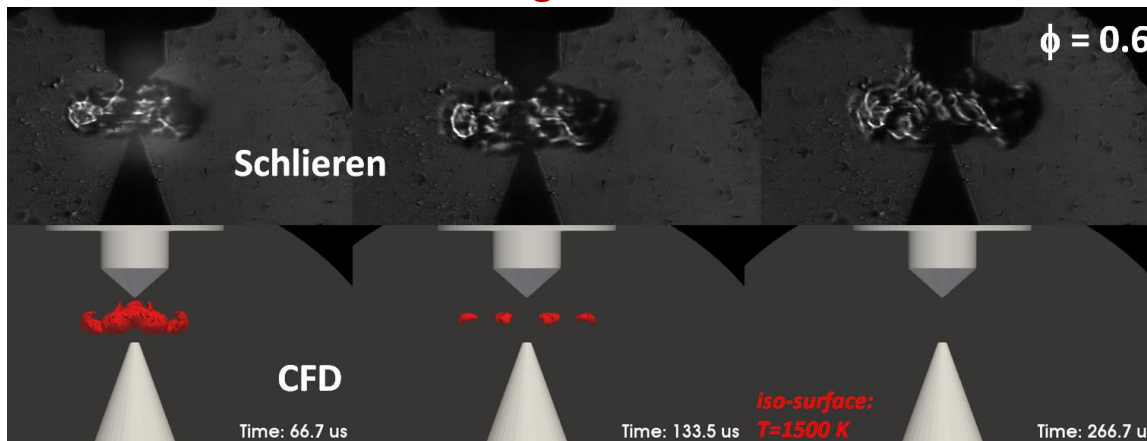
- LES dynamic structure with multi-zone finite rate chemistry.
- GRI-mech 3.0, Minimum mesh size 25 μm (AMR and embedding).
- VizSpark delivers spark-channel formation, shape, and size.
- Kernel initialization: plasma-chemical equilibrium approach.
- Energy and plasma volume used to compute chemical equilibrium.
- LESI model not needed for quiescent conditions.

SI CFD model evaluated at varying operating conditions

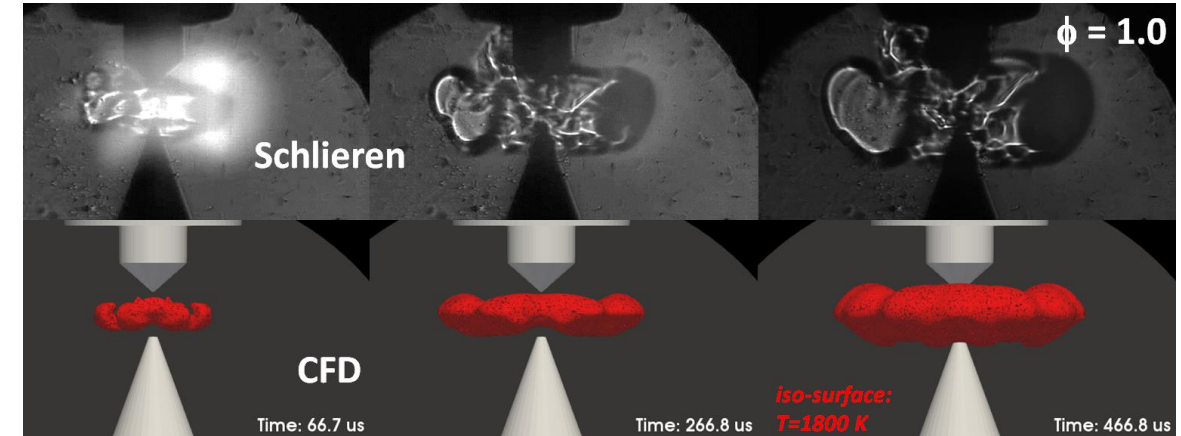
Stoichiometric condition ($\phi = 1.0$)

- Standard energy deposition approach failed, due to temperature values exceeding the limit ($\geq 95,000$ K).
- Equilibrium calculation delivered reasonable Temp values.
- Initial expansion of the flame kernel well described by CFD simulations with respect to experiments.
- Accurate energy value (4 mJ) crucial to match expansion.

Schlieren images from Ekoto, SNL



Schlieren images from Ekoto, SNL



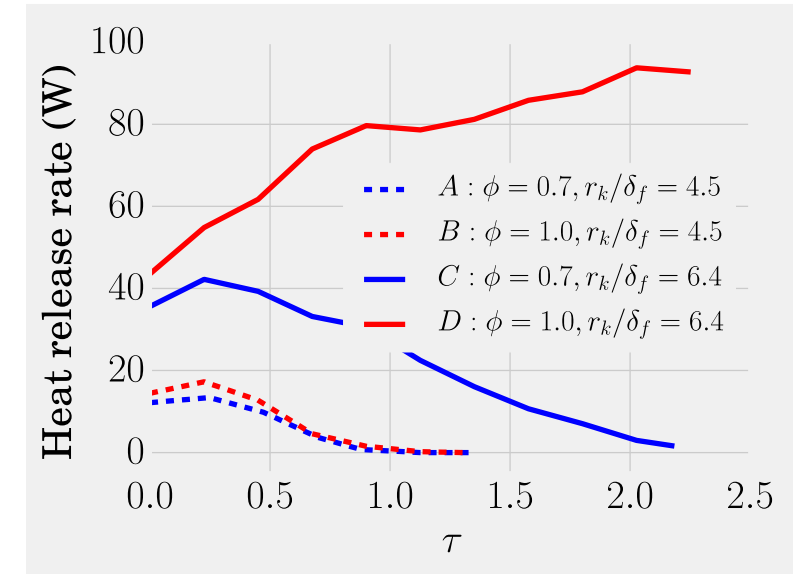
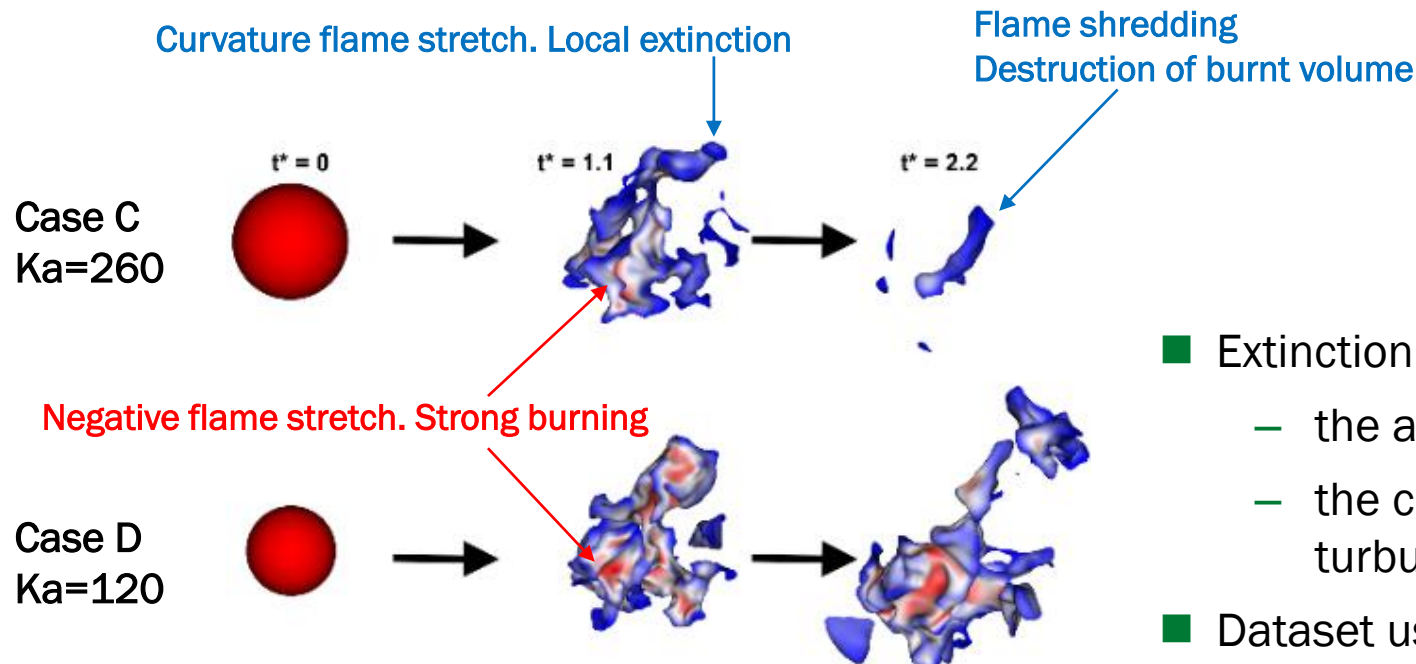
Lean condition ($\phi = 0.6$)

- Initial expansion of the flame kernel well described by CFD simulations with respect to experiments.
- CFD failed to predict successful ignition:
 - Minimum impact of heat transfer
 - Uncertainties in ϕ measurements under evaluation
 - Quenching due to flame shredding or low reactivity?

Introduce DNS to investigate flame kernel growth and develop LES sub-models

DNS of turbulent flame kernels provided for ML model training

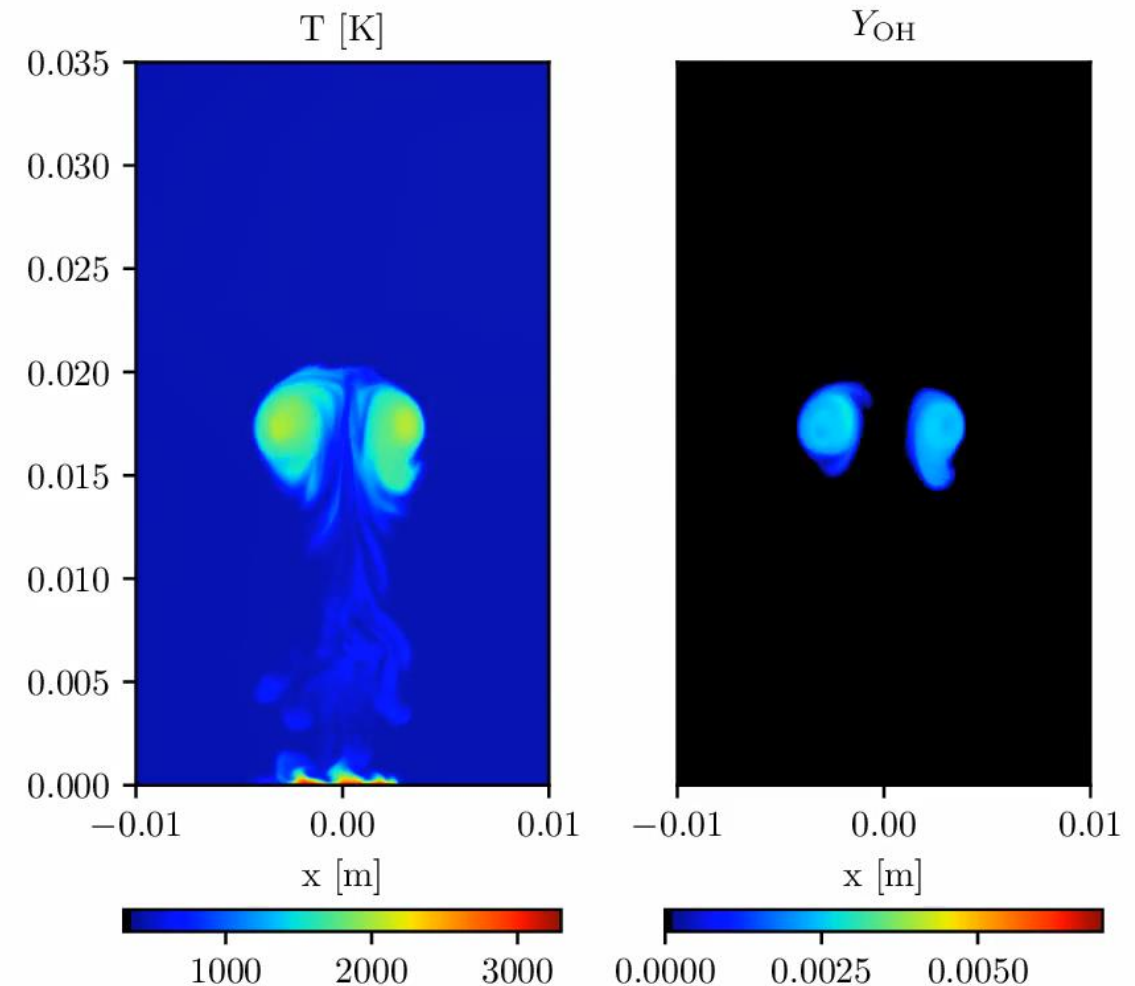
- Jet A at $\phi = 0.7-1.0$, $Ka = 120-260$, $Re_t = 2500$.
- Parametric variation with kernel size and equivalence ratio.
- Cases A, B, C global extinction. Case D marginal.



- Extinction mechanisms identified as:
 - the attenuation of local HRR due to flame stretch
 - the cut-off and destruction of burnt volume due to turbulence
- Dataset used by NREL for the ML-based manifold model.

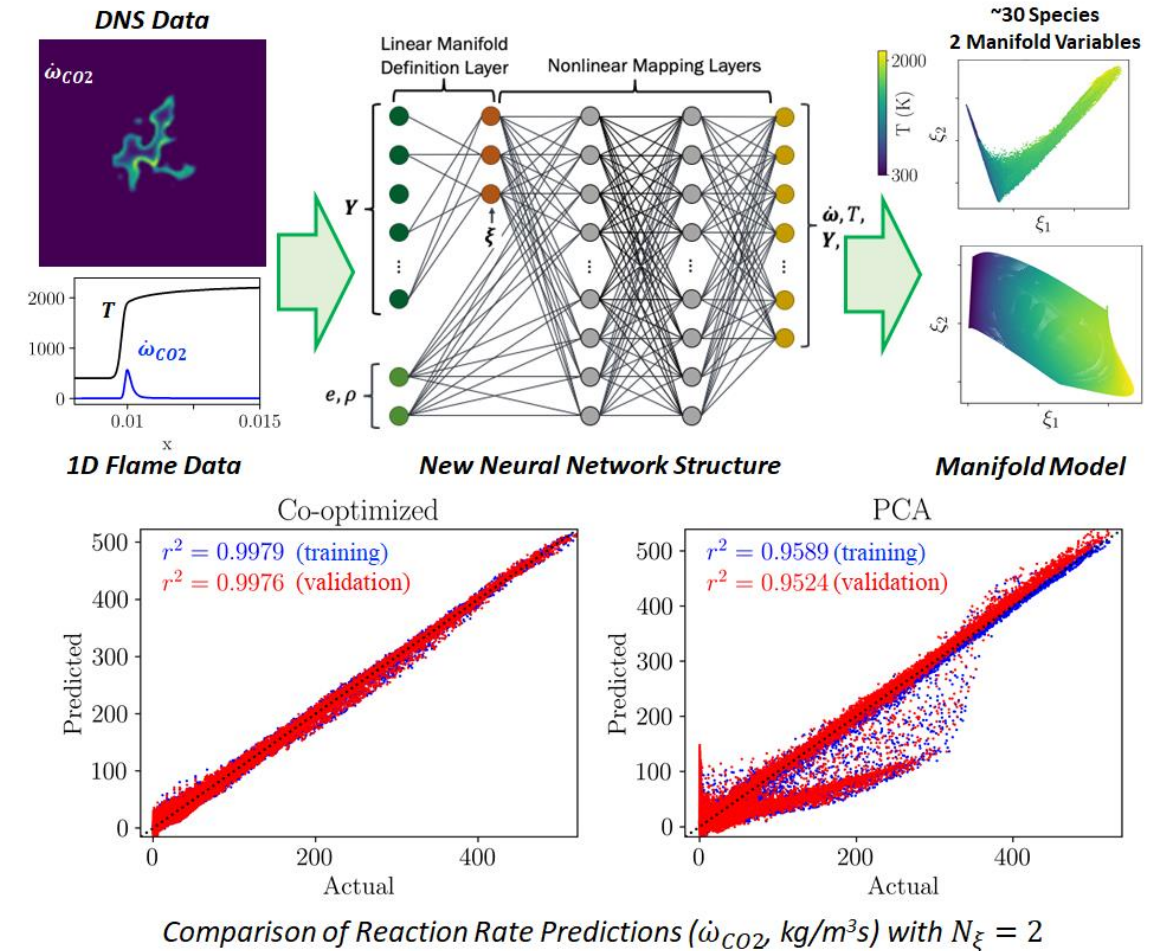
Preliminary DNS of plasma post discharge flame kernel evolution

- DNS evolution of a thermal ignition flame kernel ejected from a sunken aerospace ignitor into a quiescent methane-air mixture (Georgia Tech rig).
- Initial kernel parameters from Stanford University (Matthias Ihme) for a high-altitude relight case.
- PeleC with AMR (3 levels of refinement near kernel).
- Stoichiometric to lean mixture range covered.
- DRM-19 mech used for methane.
- Onset of ignition at very lean conditions, partially at leading edge and 'at the side' of the kernel.
- Vortex traps OH, cool air is recirculated, flame can't be sustained at the leading edge. Later on the fuel is recirculated and mixes with kernel leading to ignition.



ML-based reduced-order manifold model developed

- Reduced-order manifold approach for reaction rate and turbulence/chemistry interaction closure in LES:
 $\dot{\omega}(Y, e, \rho) = \mathbf{G}(\xi, e, \rho)$ where $N_{\xi} \ll N_Y$
- Novel neural network structure developed to simultaneously optimize both the manifold definition (ξ) and the nonlinear mapping to the model outputs (\mathbf{G}), unlike other modeling approaches.
- Model trained using the SNL Jet-A DNS and data from simple 1D and 2D calculations.
- Prediction error for reaction rates and heat release reduced relative to state-of-the-art physical and data-based models, e.g. Principal Component Analysis (PCA).
- Will lead to more accurate overall prediction of ignition when model is integrated into LES solvers.
- Training with filtered heat release rate data in progress.

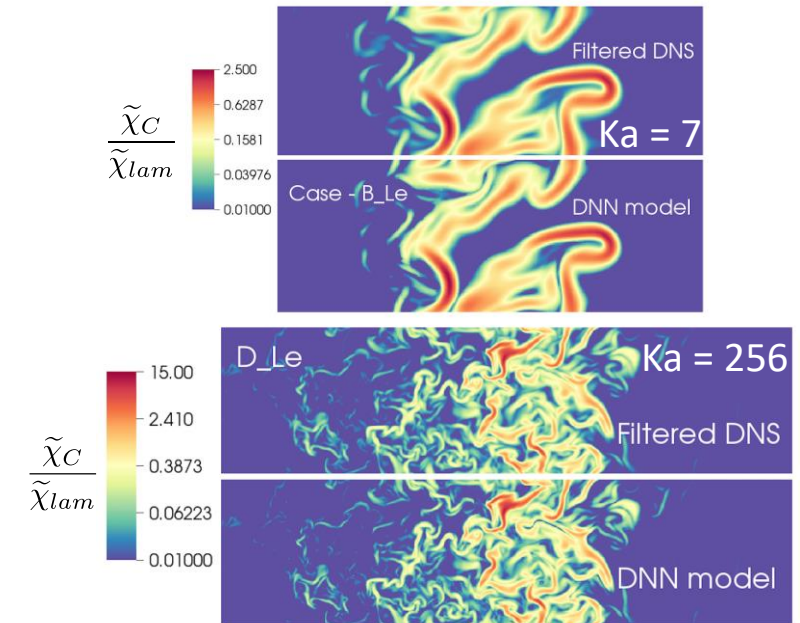


Milestone: ML-based models captured spatially filtered DNS heat release rates

ML-based model developed for progress variable dissipation rate (PDR)

- PDR, χ_c is a key modeling component of premixed turbulent combustion models. It provides information about the interplay between turbulent and flame time scales.
- Developed a Deep Neural Network (DNN) based LES model for χ_c using filtered DNS data from n-heptane flames (Caltech).
- Training data spanned varying turbulence levels and flame thickness leading to a range of Karlovitz numbers.
- In a-priori analysis model showing great promise and providing significant improvement over current state-of-art models.
- Model designed to predict:
 - a. χ_c in flames with fuels ranging from H_2 to long chain hydrocarbons such Dodecane ($C_{12}H_{26}$)
 - b. Karlovitz numbers (Ka) ranging from 0.5 to 256

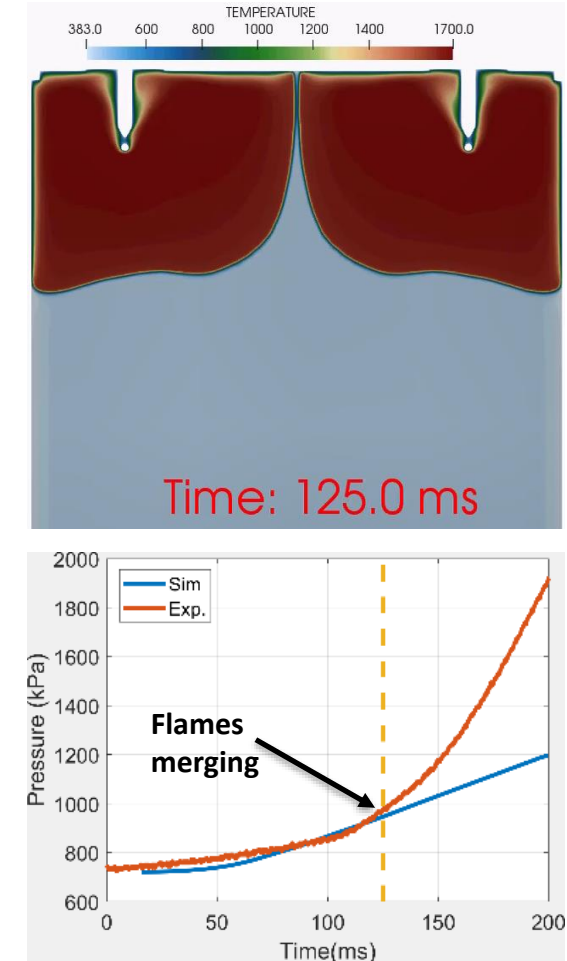
Prediction of $\tilde{\chi}_c$ from ML based model compared against filtered DNS



Milestone: ML-based models captured spatially filtered DNS heat release rates

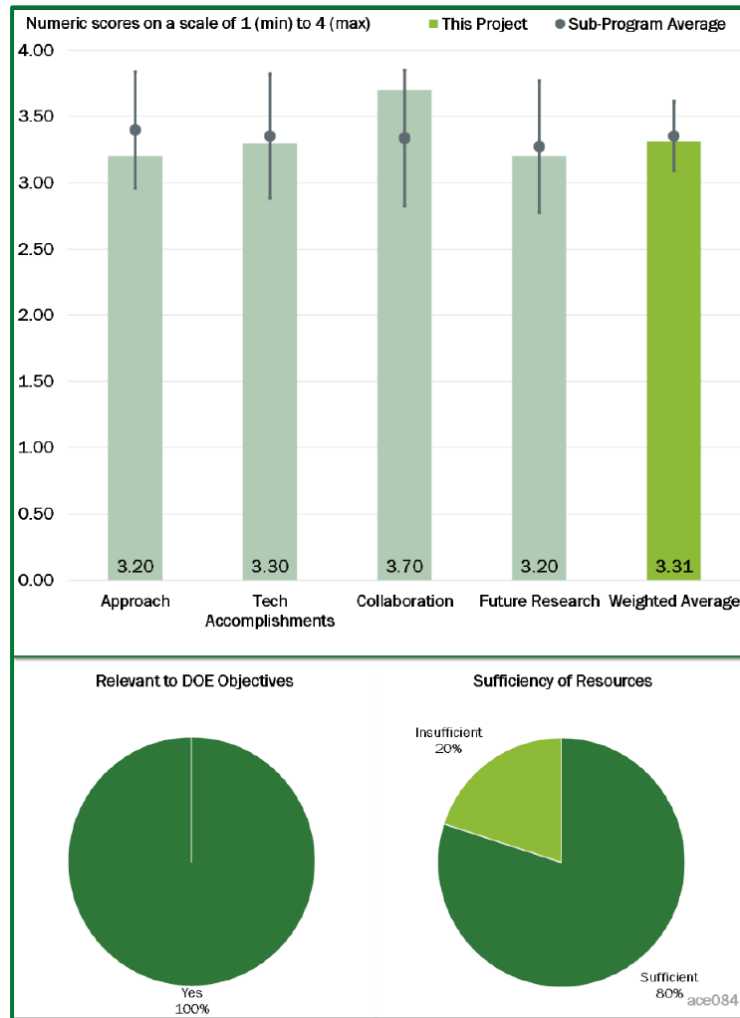
Preliminary evaluation of flame kernel merging mechanisms

- Simulation of a pre-burn event for soot wall film experiment in the Sandia constant volume chamber at quiescent condition.
- Volumetric composition: 3.2 % C_2H_2 , 0.5% H, 8.25 % O_2 , 88.05 % N_2 .
- CONVERGE SAGE solver (finite rate chemistry with multi-zone):
 - 73-species C_2H_2 mechanism. Captures differential diffusion effects
- 3 consecutive sparks with 80 mJ total energy, 12.5 ms total duration.
- Flame stabilized after 15 ms, captures propagation within the first 100 ms.
- Flame merging after 125 ms causes divergence in pressure trace agreement.
- Future focus on early flame kernel evolution and merging mechanism:
 - Scalar mixing across the flame and turbulent flame speed
 - G-equation as an effective model compared to multi-zone finite rate
 - Iso-octane and gasoline surrogate simulation to follow



RESPONSE TO REVIEWER COMMENTS

C.02.04 was the only task reviewed in FY19 (Ref. ACE084, Scarcelli, 2019)



RE-SCOPE PROJECT TO BE MORE COMPREHENSIVE AND EFFICIENT

- The reviewer wanted to see the geometry and conditions (engine speed and loads) that will be modeled and further stated that practical engine conditions (including high load) are important for industrial applications.
- The focus of the current project is very broad, possibly too broad. The project considers three modes of ignition—traditional spark ignition (SI), low-temperature plasma (LTP), and pre-chamber (PC) jet ignition.
 - ✓ 'High-fidelity' SI modeling is the main focus. LTP and PC 'engineering' models are also needed.

THE COMPLEXITY OF PLASMA CHEMISTRY

- Plasma predictive chemistry is heavily lacking; thus, this area needs much attention.
- Collaboration with Lawrence Livermore National Laboratory (LLNL) will be good for integrating with neutral chemistry, but there is a lot of expertise in the academic community for plasmas that should be leveraged more heavily.
 - ✓ Collaboration planned within PACE (LLNL) and outside of PACE (Auburn/U-Texas).

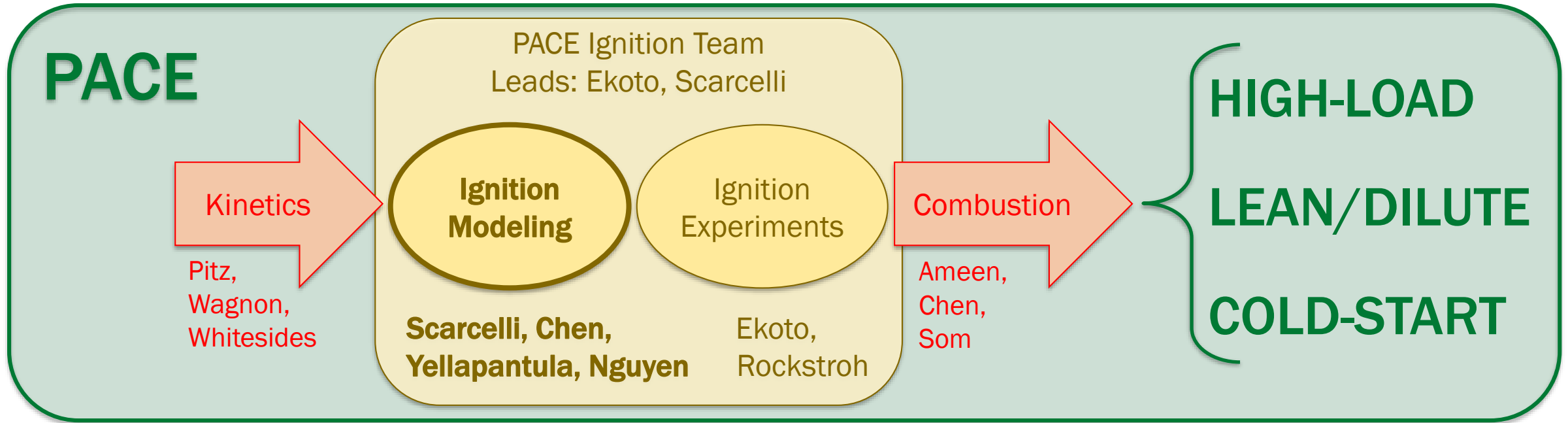
TAILORED EXPERIMENTS AND/OR DNS

- Ask if the project team could experimentally reduce some of this uncertainty with a cleverly designed experiment.
- Additional experimental data in terms of whether actually a shockwave is seen, e.g., schlieren. Additional non-intrusive temperature and species field data using optical diagnostics may be helpful in VizGlow model validation
- Wherever experimental data cannot be acquired, the reviewer recommended investigating whether direct numerical simulations (DNS) will yield any data that can be used for VizGlow validation.
 - ✓ Experiments on ignition being tailored on modeling activities. DNS is now part of our approach.

MORE EFFORT HIGH-FIDELITY CALCULATIONS

- It would be nice to have seen some preliminary comparisons with LES at the Annual Merit Review (AMR).
- Too premature to use detailed CONVERGE simulations at this point. Perhaps only LES in CONVERGE may allude to some results (less diffusion).
 - ✓ CONVERGE simulations are now being performed using LES.

COLLABORATION AND COORDINATION



EXTERNAL COLLABORATORS

Convergent Science (CSI) – *CFD model development*
Esgee Technologies – *plasma model development*
Tenneco, Transient Plasma Systems (TPS) – *ignition hardware*
Michigan Tech, U-Perugia (optical diagnostics), U-Texas,
Auburn (plasma chemistry), Purdue (combustion modeling)
FCA Group – *LES model development through CRADA*

CONNECTION WITH OTHER DOE PROGRAMS

DOE HPC4Mfg – TPS/ANL, plasma modeling
DOE TCF – CSI/ANL, LES model in CONVERGE
DOE VTO FT – ANL, Pre-chamber modeling for MD/HD
NG engines and multi-mode combustion (Co-Optima)
DOE SC ASCR ECP – SNL, Pele AMR DNS code with
igniter geometry capability

REMAINING CHALLENGES AND BARRIERS

■ Predictive ignition modeling serves multiple purposes within PACE

- Future milestones ‘weighted’ on priority, state-of-the-art, and computational requirements.
- Model limitations well-known at high-load and lean/dilute conditions. Cold-start is unclear.

■ Conventional vs. non-conventional ignition systems

- Can afford fundamental-to-applied modeling only for a limited number of ignition concepts.
- SI has priority. PC or LTP modeling might just remain at the engineering level in FY21-23.

■ Computational resources for DNS are limited

- DNS-based model development can fit into all three main purposes.
- High-load conditions will face more severe time constraints due to high turbulence.

■ Will reduced kinetics be reduced enough?

- Kinetic mechanisms needed in different sizes. DNS has the largest constraints.

PACE-wide barriers are discussed in ACE138

PROPOSED FUTURE WORK

COV: Coefficient of Variation

■ Multi-Lab effort on predictive Spark-Ignition model development

- Involving all PIs/Tasks. ANL also involved in CRADA with FCA (LESI model development)
- 3-pronged approach: plasma discharge → DNS of kernel → flame growth sub-models
- Specific purposes subsequently targeted, based on readiness and challenges:
 - Lean/Dilute: FY20-FY21
 - Cold-Start: FY21-FY22
 - High-Load: FY21-FY23

■ Develop engineering CFD models for advanced ignition systems

- ANL will continue to develop and improve ‘engineering-level’ CFD models for PC/LTP
 - PC will surely leverage advances in SI modeling and combustion modeling
 - LTP will take longer due to complex plasma discharge-to-kernel kinetics
- Impact of advanced ignition on cold-start and ACI COV stability evaluated in FY22 and FY23

Any proposed future work is subject to change based on funding levels

SUMMARY

Development and Validation of Simulation Tools for Advanced Ignition Systems

Relevance

- This project addresses the lack of predictive models for conventional and non-conventional ignition processes and limited understanding of advanced ignition mechanisms for high-efficiency engines

Approach

- Three-pronged approach consisting of high-fidelity plasma modeling, DNS/experiments of flame kernel initiation and growth, and physics-based or ML-based LES ignition sub-model development

FY20 technical accomplishments (1/2)

- Ignition modeling tools (plasma, CFD, kinetics) improved and expanded
- Improved characterization of discharge-to-plasma simulations
- RF corona plasma simulated and validated against experiments
- Engineering-level TPI model for CFD solvers developed
- SI kernel growth simulated with CFD and compared with experiments
- SI CFD model evaluated at varying operating conditions

FY20 technical accomplishments (2/2)

- DNS of turbulent flame kernels provided for ML model training
- Preliminary DNS of plasma post discharge flame kernel evolution
- ML-based reduced-order manifold model developed
- ML-based model developed for progress variable dissipation rate
- Preliminary evaluation of flame kernel merging mechanisms

Remaining barriers

- Broad ignition work target identified by multiple purposes in PACE
- Focus on conventional vs. non-conventional ignition systems
- Computational resources required for DNS and size of mechanisms to be used by DNS and engineering-level CFD models

Future work

- Multi-Lab effort on predictive spark-ignition model development
 - Addressing lean/dilute, cold-start, and high-load ignition
- Develop engineering CFD models for advanced ignition systems

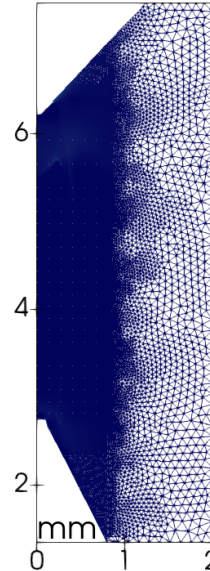
TECHNICAL BACKUP SLIDES

LTP ignition simulation setup

VizGlow

Self-consistent non-equilibrium plasma solver that describes streamer discharge:

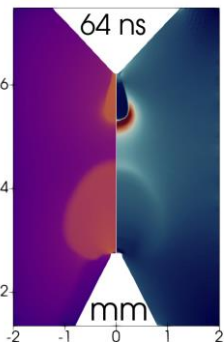
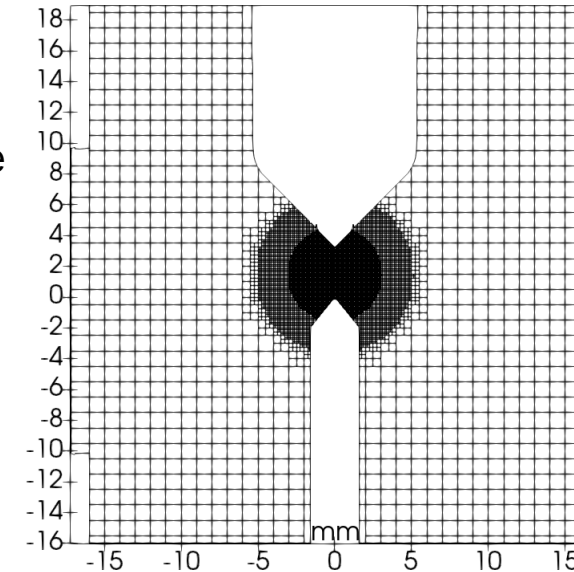
- 2D axisymmetric. 10 μm min mesh size
- Chemistry: air-plasma [Zhang et al., 2018](#)
- Gas: pure air at 343 K, 1.3 bar
- BCs: Voltage profile from post-processed experimental data imposed to the anode
- 1-pulse simulation conducted; 2nd pulse fields based on the assumption that a plasma kernel of density 10^{18} 1/m^3 exists.



CONVERGE CFD

CFD software for engine simulation

- Turbulence: LES Dynamic Structure
- Chemistry: Reduced mechanism from USC (propane)
- Grid control:
 - Base size: 2 mm
 - Embedding: 125 μm
 - AMR: 125 μm
- BCs: fixed wall temperature



Step 1:

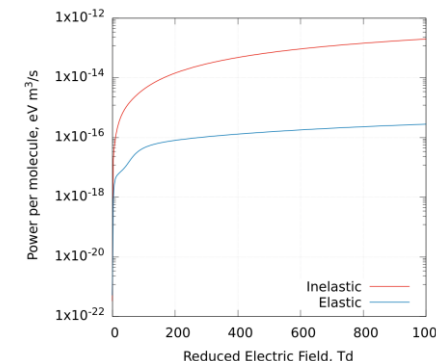
VizGlow
discharge
simulation
 $t \sim 100\text{ns}$

Step 2:

Power
deposited for
each domain
cell

Step 3:

[Bolsig+](#) calculations
of elastic (heat) and
inelastic (radicals)
collisions



Step 4:

Source terms for
governing
equations in
CONVERGE via
UDFs

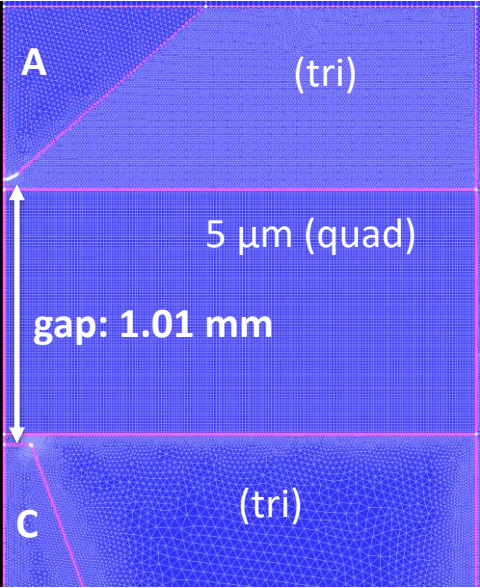
Spark plasma and ignition kernel growth simulation setup

CHT: Conjugate Heat Transfer

VizSpark

Self-consistent equilibrium plasma solver that describes the evolution of spark-ignition processes

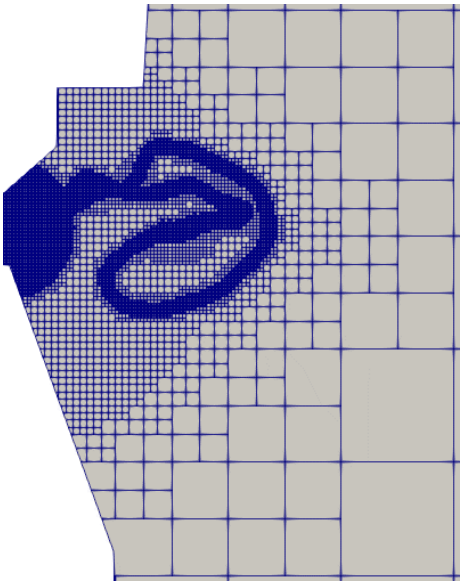
- 2D axisymmetric solution
- Min mesh size: 5 μm
- Chemistry: air-plasma
- Gas: pure air at 343 K, 5 bar
- BCs: Current density profile from post-processed experimental data is imposed to the cathode



CONVERGE CFD

CFD software for engine simulation

- Turbulence: LES Dynamic Structure
- Chemistry: GRI-Mech 3.0 (methane)
- Grid control: Base size: 1.6 mm. Embedding: 25 μm , AMR: 25 μm
- BCs: fixed wall temperature
- CHT calculations not needed due to short spark duration and toroidal kernel shape growth



Step 1:

Obtain plasma channel thickness from VizSpark

Step 2:

Equilibrate air by maximizing entropy isochorically with given measured energy and plasma volume

Step 3:

Equilibrate fuel-air mixture by minimizing Gibbs free energy isobarically

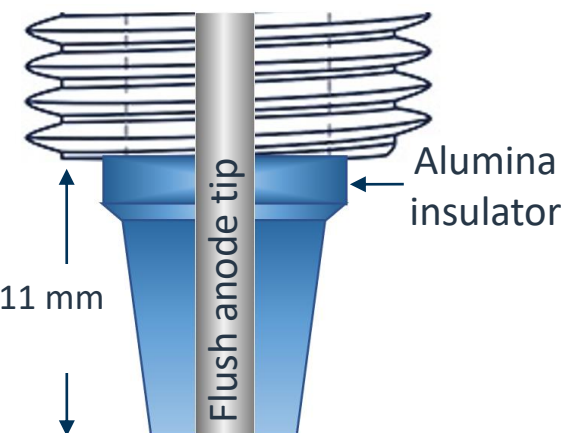
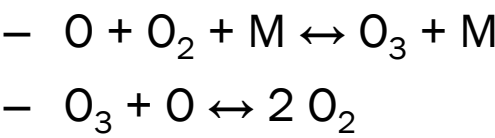
Step 4:

Initialize equilibrated T, P, Y_i in CONVERGE

Methodology	Description	<div><div>* estimation</div><div>** cylinder diameter from VizSpark simulation</div></div>							
Standard ED	Sourcing the measured power [J/s] along a cylindrical volume between gap*								
Plasma-chemical equilibrium	Initializing the equilibrated temperature, pressure, species mass fractions along a cylindrical volume between gap**								
	- Temperature: ~25,700 K; Pressure: ~990 bar								
	- Species mass fraction (for phi=0.6 case):								
	N	0.739	O	0.224	C	0.025	H	0.008	
	N2	0.002	O2	4.1e-5	CO	5.0e-5	H2	3.2e-6	
	NO	0.001	OH	7.1e-5	CO2	5.9e-9	H2O	1.1e-19	
					CH4	2.9e-8	HO2	1.0e-16	

ANL tools: details and references

- Circuit modeling conducted via [Screamer](#).
- Ozone mechanism used for ignition and propagation studies: Ombrello et al. ["Flame propagation enhancement by plasma excitation of oxygen"](#)
- Propane mechanism used for flame propagation: Kennel et al. ["Reduced kinetic mechanisms for premixed propane-air flames"](#)
- Propane mechanism used for ignition studies: Reduced USC Mech: [Website](#)
- Flame propagation conducted with [Basilisk](#) and [Cantera](#) routines
- Simplified Ozone mechanism used in VizGlow GBDI calculations: Depcik et al.: [Website](#)



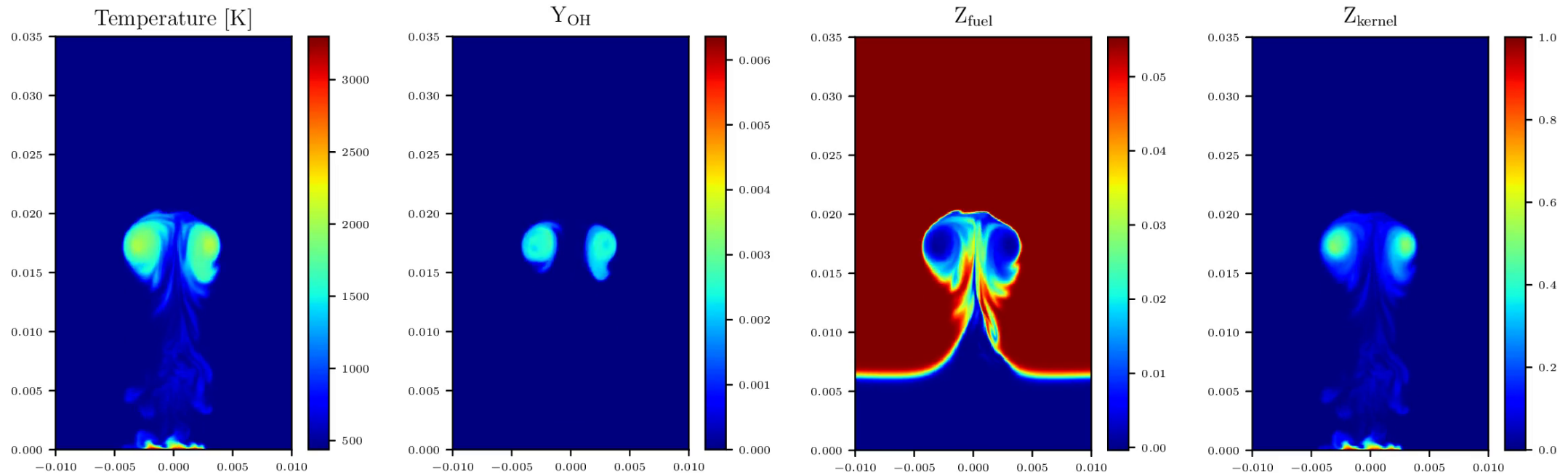
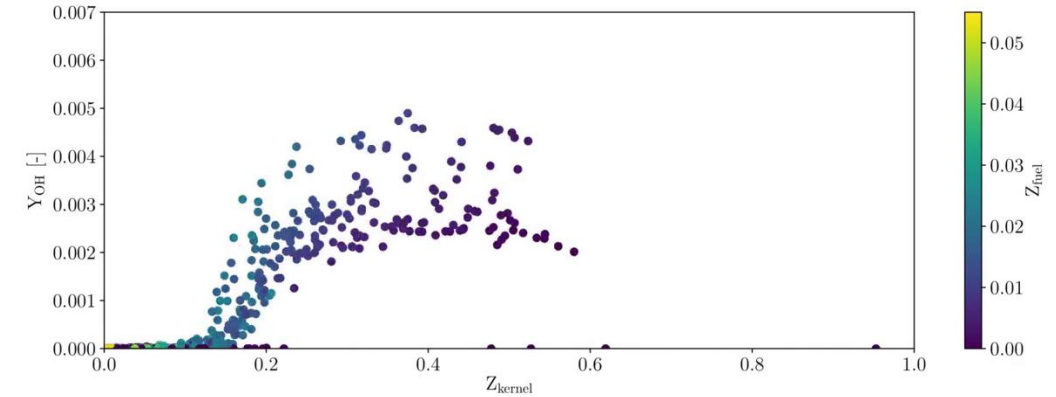
ASSUMPTIONS FOR OZONE GBDI CALCULATIONS

- Simulations run VIZGLOW on two-pulses in rapid succession without dwell time
- Experiments performed at SNL divided total ozone generation (on 10 pulses) by 10

	Simulations	Experiments
1 pulse	$X_{O_3} = 3.13 \text{ ppm}$	$X_{O_3} = 3.75 \text{ ppm}$
2 pulses	$X_{O_3} = 8.87 \text{ ppm}$	$X_{O_3} = 7.51 \text{ ppm}$

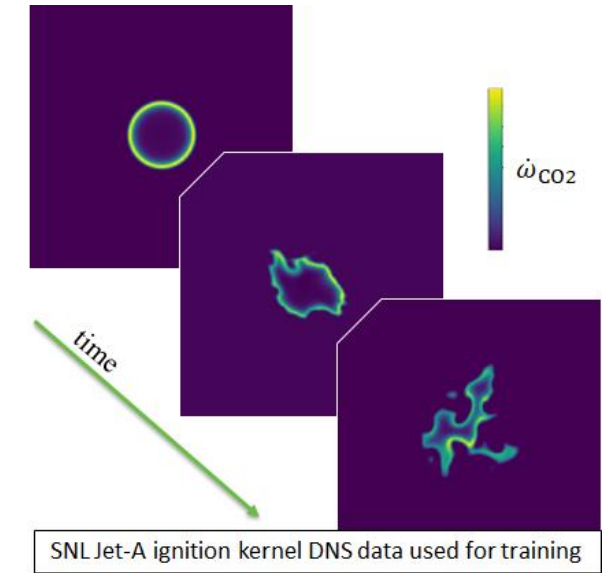
DNS of plasma post discharge flame kernel evolution

- Onset of ignition at very lean conditions, partially at leading edge and 'at the side' of the kernel
- Vortex traps OH, cool air is recirculated, flame can't be sustained at the leading edge. Later on the fuel is recirculated and mixes with kernel leading to ignition



Machine Learning (ML) models - Technical approach

- A key challenge for all LES models is closure of the filtered reaction rates ($\tilde{\omega}_k$) based on filtered thermochemical state variables
 - *Reduced-Order Manifold Models*: solve for reaction rates based on the progress variable (e.g., $C = Y_{\text{CO}_2} + Y_{\text{CO}} + Y_{\text{H}_2\text{O}} + Y_{\text{H}_2}$), rather than all species individually
- Deep neural networks (DNNs) efficiently represent complex nonlinear relationships
- Two approaches for integrating DNNs to leverage DNS and experimental data to accurately predict the impact of turbulence on the filtered reaction rates:



Machine Learned Manifold

- Use a specifically designed neural network structure to learn new manifold variables rather than using the same progress variable
- This approach gives both the *functional form* of the model for $\tilde{\omega}_k$ and the *inputs* to the model

Progress Variable Manifold w/ DNN Sub-model

- *Progress variable dissipation rate* (χ_c) is a key model parameter that indicates the turbulence intensity and effect on combustion
- A DNN model for this quantity can improve accuracy over phenomenologically derived approaches

Objective: Improved kernel-to-flame transition model that accounts for plasma energy deposition, hydrodynamic instabilities, turbulence, convective strain, electrode heat transfer, and fuel Lewis number